### KaSim reference manuel

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## Contents

1	Introduction	5
2	Installation	7
3	The command line	9
4	The kappa file	11
Bibliography		13



#### Introduction

KaSim is an open source stochastic simulator of rule-based models [3, 2, 4] written in the  $\kappa$ -calculus. Basically KaSim takes one or several kappa files as inputs and generates stochastic trajectories of various observable. KaSim implements the network free simulation algorithm for rule-based models [1] that extends Gillespie's algorithm [5, 6].

A simulation event corresponds to the application of a rewriting rule, contained in the kappa file, to the current graph (also called a mixture). The rule is selected according to its activity, i.e the number of instances it has in the current mixture, multiplied by its kinetic rate, and applied one of its possible instance in the graph. It results in a new graph together with an updated activity for all rules (see Fig. 1.1).

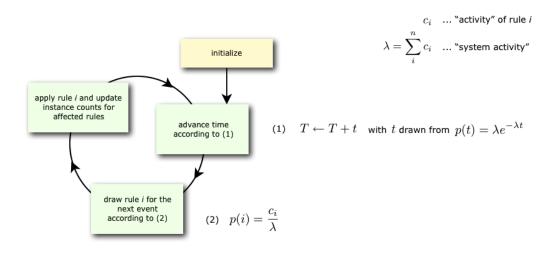


Figure 1.1: The event loop



Importantly, the cost of such an event is independent of the size of the graph it is applied to [1]. Note that KaSim is not equipped with a curve visualization tool. However, the outputted data are in text format and usable with any standard plotting software such as GnuPlot.

#### Installation

To obtain KaSim you can either use pre-compiled binaries available on KappaLanguage.org or compile the sources for your architecture. To do so, download the source code from https://github.com/jkrivine/KaSim and make sure you have a recent ocaml compiler installed. From a terminal window type ocamlopt.opt -v. If nothing appears then you need to install Ocaml Native compiler that can be downloaded from http://caml.inria.fr/download.en.html.

Once Ocaml is safely installed, untar KaSim archive and compile following these few steps:

```
$ tar xzvf kasim.tar.gz -d Kappa
$ cd Kappa
$ make
```

At the end of these steps you should see, in the Kappa directory, an executable file name KaSim. In order to check the compilation went fine, simply type .\KaSim --version. If the ocaml native compiler ocamlopt.opt is not in the path of your system, you may set the variable OCAMLBINPATH to point to the location of the compiler by editing the corresponding line in the Makefile.



The command line



The kappa file



## **Bibliography**

- [1] Vincent Danos, Jérôme Féret, Walter Fontana, and Jean Krivine. Scalable simulation of cellular signaling networks. In *Proceedings of APLAS'07:* 5<sup>th</sup> ASIAN symposium on programming languages and systems, volume 4807 of LNCS, pages 139–157, 2007. Invited paper.
- [2] Vincent Danos, Jérôme Feret, Walter Fontanta, Russ Harmer, and Jean Krivine. Rule based modeling of biological signaling. In Luís Caires and Vasco Thudichum Vasconcelos, editors, *Proceedings of CONCUR 2007*, volume 4703 of *LNCS*, pages 17–41. Springer, 2007.
- [3] Vincent Danos and Cosimo Laneve. Formal molecular biology. *Theoretical Computer Science*, 325, 2004.
- [4] James R. Faeder, Mickael L. Blinov, and William S. Hlavacek. Rule based modeling of biochemical networks. *Complexity*, pages 22–41, 2005.
- [5] Daniel T. Gillespie. A general method for numerically simulating the stochastic time evolution of coupled chemical reactions. *Journal of Computational Physics*, 22(4):403– 434, 1976.
- [6] Daniel T. Gillespie. Exact stochastic simulation of coupled chemical reactions. *Journal of Physical Chemistry*, 81(25):2340–2361, 1977.